

Improved Prediction of Hydraulic Conductivity with Soil Water Retention Curve that Accounts for Both Capillarity and Adsorption Forces

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Abstract

Hydraulic conductivity curves (HCCs) are important parameters in land surface modeling. The general way for predicting HCC from soil water retention curve (SWRC) requires an additional input of the saturated hydraulic conductivity. The time-consuming in measurement and more importantly, the macro-effect near saturation, however, often result in difficulty and poor performance in predicting the conductivity. In this study, we provided a physically based method for predicting the HCC fully from SWRC requiring no additional parameters. This is achieved by applying an estimated conductivity (from SWRC) in the dry range as new matching point, in together with modifying the HCC model developed by Wang et al. (2018) that accounts for both capillarity and adsorption forces. Testing with a total of 159 soil samples yielded that the new model significantly improved the predictions of HCC, with R^2 being 0.74 and root mean value being 0.84 cm d^{-1} , nearly double and half of the value predicted with the input of the saturated hydraulic conductivity, respectively. The abrupt drop near saturation of the HCC model that provided by Wang et al. (2018) for soils with small n values close to 1, a parameter in shaping the SWRC, was also overcome by introducing a non-zero air-entry value.

1. Introduction

Hydraulic conductivity properties are frequently required in water and solute transport simulation. Due to the difficult and time-consuming in measurement, in general, the hydraulic conductivity curve (HCC) is physically or empirically related to, and then can be predicted from the soil water retention curve (SWRC) through the integration of flux in a bundle of capillary tubes (e.g., Burdine, 1953; Mualem, 1976; Alexander & Skaggs, 1986). Among them, the most popular one might be the framework provided by Mualem (1976). Specifically, this built relationship is for the relative hydraulic conductivity. To describe the actual HCC, a matching point, usually taken at the saturated hydraulic conductivity K_s , is required.

Besides the time-consuming in measurement for especially large-scale applications, the usage of K_s as matching point, in spite of the wide acceptance, can cause significant deviation from unsaturated conductivity observations. Schaap and Leij (2000) and Schaap et al. (2001) demonstrated that applying observed K_s as matching point leads to overprediction of conductivities at most matric potentials. The reason, as discussed in detail by van Genuchten and Nielsen (1985), is that the K_s is sensitive to macropore flow while unsaturated flow occurs in the soil matrix. van Genuchten and Nielsen (1985) therefore argued that the matching point, ideally should be located at a point below saturation.

The advances in soil hydraulic properties modelling suggested that by including the impact of adsorption forces, the developed models can well describe the soil hydraulic properties from saturation to oven-dryness (e.g., Tuller & Or, 2001; Lebeau & Konrad, 2010; Wang et al., 2013; 2016). In the dry range where adsorption forces dominate, the unsaturated hydraulic conductivity is controlled by the film thickness and the specific surface area (Bird, 1960; Tokunaga, 2009). As the film thickness can be estimated from matric potential (Tokunaga, 2009; 2011) and the specific surface area estimated from soil water retention curve (Tuller & Or, 2005), the hydraulic conductivity that accounts for adsorption forces thus can be directly estimated from the known soil water retention curve. This method, firstly provided by Lebeau and Konrad (2010), showed very good performance in hydraulic conductivity estimation in a series of applications (Wang et al., 2017; 2018; 2019). Therefore, it is wonder that if the estimated conductivity under dry conditions can be applied as a better matching point than K_s in hydraulic conductivity prediction.

To apply the estimated conductivity under dry conditions as the matching point, the hydraulic conductivity function, however, must capture the impact of capillarity and adsorption forces in a continues formular. The combination models as presented in (e.g., Lebeau & Konrad, 2010; Zhang, 2011; Wang et al., 2016; Liao et al., 2018; Stanić et al., 2020 among others) used different formular to describe the capillarity- and adsorption-associated conductivities, respectively. The conductivities in the wet range showed no tight connection with those in the dry range. For these combined models, the estimated conductivity under dry conditions thus cannot be applied as the matching point.

Different from these developed models that treat the total conductivity as a sum of the capillary one and the non-capillary one, Wang et al. (2018) presented a continues formular to describe the HCC over the entire moisture range. It showed a similar form with the commonly used van Genuchten (1980) -Mualem (1976) model (hereafter referred to as the VGM model) and required no additional parameters in predicting the HCC. The HCC is written as

where h_0 is the matric potential corresponding to the zero water content and is set as -6.3×10^6 cm according to Schneider and Goss (2012), l is an empirical factor and has a typical value of 3.5 as suggested by Wang et al. (2018), $\Gamma(h)$, m , n are parameters in relation with the soil water retention curve that provided by Fredlund and Xing (1994), written as

where $S = \theta / \theta_s$ is the saturation degree with θ ($\text{L}^3 \text{L}^{-3}$) being the volumetric water content and θ_s ($\text{L}^3 \text{L}^{-3}$) being the saturated water content, h (L) is the matric potential, h_r is interpreted originally as the matric potential corresponding to the residual water content by Fredlund and Xing (1994). For not applying the definition of the so-called residual water content, h_r is simply regarded as a shape parameter and is set as -1.5×10^3 cm following Fredlund and Xing (1994). It should be noted that h_r is incorrectly written as -1.5×10^2 cm in the text in Wang et al. (2018), although the performance of equation (2) is not sensitive to the value of h_r (Wang et al., 2017). And $\Gamma(h)$ is written as

with Γ (L^{-1}) being the fitted parameter.

Equation (1) shows that with estimated hydraulic conductivity in dry range, the K_s and then the HCC can be predicted because all other parameters required are determined from the known SWRC (equation 2).

In addition, the original HCC provided by Wang et al. (2018) does have one limitation. That is, the HCC described in equation (1) would drop abrupt near saturation and yielded poor agreement with observations when the parameter n approaching the lower limit of 1 (Wang et al., 2018; de Rooij et al., 2021). This shortcoming, which is frequently seen in soil hydraulic models, resulting from the non-zero d/dh at the matric potential of zero (van Genuchten & Nielsen, 1985; Schaap & van Genuchten, 2006; de Rooij et al., 2021). The non-zero slope at saturation (means zero air-entry value) implies the existing of infinite pores, which is unrealistic. For the VGM model, a simple solution as provided by Vogel et al. (2000) and Ippisch et al. (2006) is to introduce a non-zero air-entry value, above which the water content is constrained to be the saturated one.

Therefore, it is the aim of this study to (1) apply the simple method that provided by Vogel et al. (2000) and Ippisch et al. (2006) to improve the prediction of hydraulic conductivity with the Fredlund and Xing (1994)-Wang et al. (2018)'s model for soils with small n values; and (2) to test the assumption that if the estimated conductivity in dry range can be treated as a matching point for HCC prediction.

2. Methods and Materials

2.1. Improved description of soil hydraulic conductivity near saturation

Following Vogel et al. (2000) and Ippisch et al. (2006), an air-entry value of h_s was introduced here to improve the performance of the Fredlund and Xing (1994)-Wang et al. (2018) model (namely as the FXW model hereafter) near saturation.

The modified SWRC of the FXW model is written as

with $\Gamma(h_s)$ being

The modified HCC of the FXW model is expressed as

When h_s has the value of 0, the SWRC and the HCC as described in equations (4) and (6) reduce to the original FXW model.

An illustration in Figure 1 (b) and (d) shows that when n value approaches the lower limit of 1, the HCC of the original FXW model drops dramatically just below saturation. For example, a tiny decrease of saturation degree just below saturation for n being 1.1 resulted in a significant decrease of relative hydraulic conductivity from 1 to about 0.2. This unrealistic decrease coming from model structure thus would underestimate the conductivities. To overcome this shortcoming, Wang et al. (2018) suggested to set a lower boundary of 1.2 for parameter n , which, however, would loss accuracy in describing the SWRC.

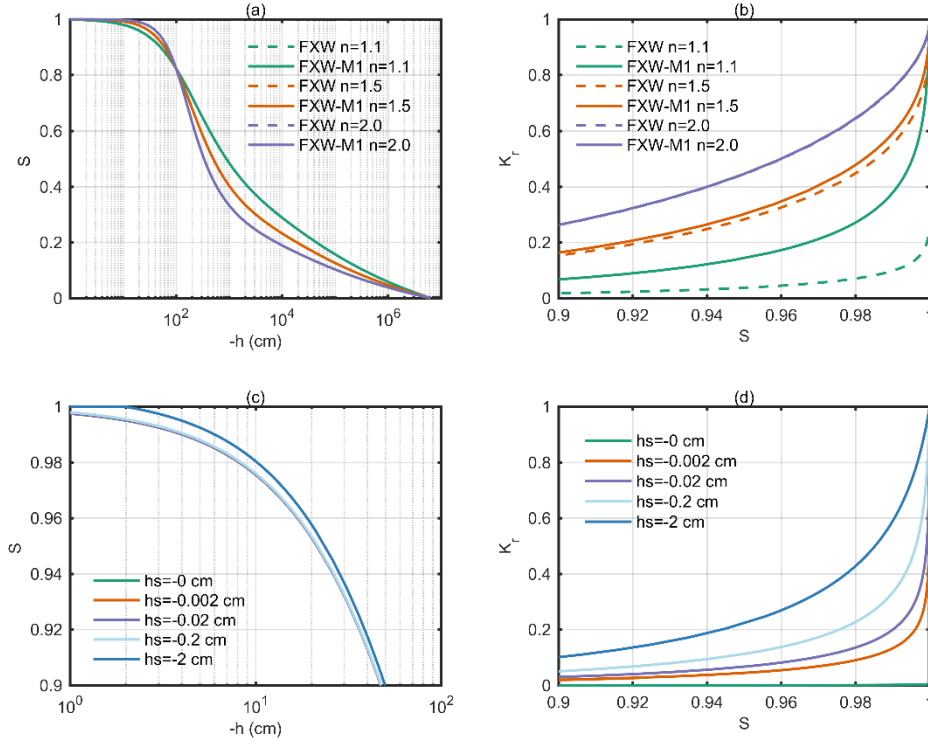


Figure 1. Illustration of the modified FXW-M1 model. (a) and (b) represents the impact of different n values on the SWRC and the HCC, respectively, where h_s is set as -0.2 cm. (c) and (d) represents the impact of different h_s on the SWRC and the HCC, respectively, where n is set as 1.01.

Here, by introducing a non-zero air-entry value, the HCC of the modified FXW model presented a much smooth decrease. For small n values close to 1, the difference between the modified model and the original FXW model is significant. While for large n close to about 2, the difference between these two models

becomes negligible (Figure 1 b).

Figure 1 (d) indicated that the improved description of HCC near saturation can be achieved with h_s value only slightly less than 0. The more negative h_s , the smoother the drop of HCC near saturation. When come to SWRC, the more negative h_s , however, yields non-decreasing water content over a longer matric potential range. For example, by setting h_s as -2 cm following Vogel et al. (2000), the modified SWRC described in equation (4) deviated significantly from the original FXW model near saturation (Figure 1 c). The modified SWRC described in equation (4) does have one limitation, that is, its derivative form is discontinue at the matric potential of h_s , which may lead to difficulty in numerically solving the Richards' equation.

Since the modified SWRC yields almost the same as the original FXW model (Figure 1 a and c) for h_s value closes to 0, therefore, different with Vogel et al. (2000), we suggested to set h_s as higher as -0.2 cm in this study. With this h_s value, the original SWRC provided by Fredlund and Xing (1994) can still be applied and has no shortcoming of discontinuity. The HCC was described by equation (6), which showed a smooth decreasing near saturation for soils with small n values (Figure 1 b and d). This modified model is namely as the FXW-M1 model hereafter.

2.2. Estimation of the new matching point from SWRC

The hydraulic conductivity that accounts for adsorption forces is determined by the specific surface area S_A ($L^2 L^{-3}$) and the film thickness f (Bird, 1960). It can be expressed as (Wang et al., 2017; Lebeau & Konrad, 2010)

with ρ being the water density ($9.98 \times 10^2 \text{ kg m}^{-3}$), g being the acceleration of gravity (9.81 m s^{-2}) and η being fluid viscosity ($1.005 \times 10^{-3} \text{ Pa s}$ at 293 K). $B(f)$ is introduced as a correction factor that accounts for the modified viscosity for film thickness thinner than 10 nm (Or & Tuller, 2000; Lebeau & Konrad, 2010). It is expressed as

with a being $5.53 \times 10^{-10} \text{ m}$ at 293 K and $\text{Ei}(-x) = -\int_x^\infty \left[\frac{\exp(-t)}{t} \right] dt$ being the exponential integral.

The film thickness f is controlled by both the electrostatic forces and the van der Waals forces, and is expressed as

with $h_e(f)$ accounts for the impact of the electrostatic forces, written in (Langmuir, 1938; Tokunaga, 2009)

with ϵ_r being the relative permittivity of water (78.54), ϵ_0 being the permittivity of free space ($8.85 \times 10^{-12} \text{ C}^2 \text{ J}^{-1} \text{ m}^{-1}$), k_B being the Boltzmann constant ($1.381 \times 10^{-23} \text{ J K}^{-1}$), T being the Kelvin temperature, z being the ion valence, set as 1 in this study, and e_c being the electron charge ($1.602 \times 10^{-19} \text{ C}$).

And $h_{van}(f)$ represents the impact from the van der Waals forces, expressed as (Iwamatsu & Horii, 1996)

where A_{svl} is the Hamaker constant for solid-vapor interactions, setting as -6.0×10^{-20} J following Tuller and Or (2005).

The S_A in equation (7) can be approximately estimated by dividing the soil water content by the film thickness as suggested by Tuller and Or (2005), assuming the soil water content is totally in film form under very dry conditions. Here, taken a typical matric potential h_m where the van der Waals forces dominate, the specific surface area can be estimated as (Tuller & Or, 2005)

With substitution of all the parameters, the calculated hydraulic conductivity by equation (7) reduced to

with $b(h_m)$ being 2.693×10^{-6} cm d⁻¹ at the matric potential h_m of -1.0×10^5 cm. When known SWRC, $K(h_m)$ can be directly estimated.

2.3. Prediction of HCC from SWRC with new matching point

With predicted $K(h_m)$, K_s therefore can be estimated by substituting equation (13) into equation (6), yields

With substitution of equation (14), the HCC as described in equation (6) thus can be described as

Compared to equation (6), the new HCC described in equation (15) requires no additional parameter other than those applied in describing SWRC (l has a constant value of 3.5). That is, the new HCC can be fully predicted from SWRC as presented in equation (2). An illustration of the new model, termed as FXW-M2, yields that the predicted conductivity in dry range is mainly controlled by the corresponding water content, that is the higher water content the higher conductivity value (Figure 2). In the wet range, in contrast, the predicted conductivity is generally much higher for coarse-textured soils.

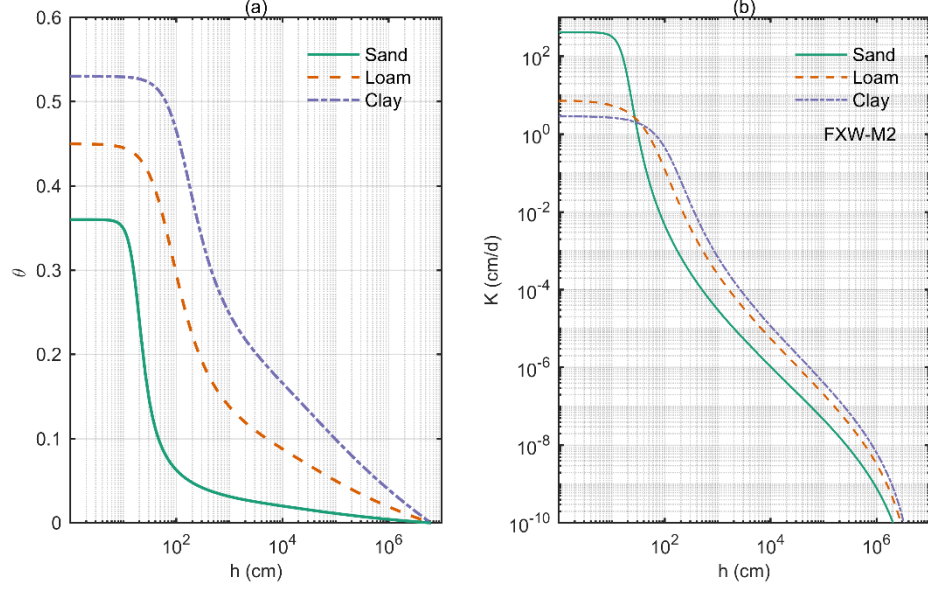


Figure 2. Illustration of the FXW-M2 model for different soil types.

2.4. Parameter Optimization

Firstly, the SWRC as described in equation (2) was optimized to derive the parameters. The objective function to be minimized is defined as

where n is the number of data pairs for the retention, θ_i and $\hat{\theta}_i$ are the measured and the simulated water content, respectively. $b = (\theta_s, n, m, \theta_s)$ is the parameter vector used for optimization, and l is set as 3.5 as suggested by Wang et al. (2018).

For parameter optimization, a low boundary of 1.01 was set for n and an upper boundary of 1.5 was chosen for m as suggested by Wang et al. (2016). The optimization was done by applying the SCE-UA method (shuffled complex evolution method developed at The University of Arizona) proposed by Duan et al. (1992).

Secondly, the HCCs as described in equations (6) and (15) were predicted with the determined parameters. It should be noted that for equation (6), the observed saturated conductivity K_s is required as input.

To evaluate the model performance, the root mean square error ($RMSE$), and the coefficient of determination (R^2) were introduced.

The $RMSE$ is defined as

with N being the number of data pairs, and θ_i and $\hat{\theta}_i$ being the measured and estimated value, respectively.

And R^2 is defined as

with \bar{o} being the mean value of o_i .

2.5. Datasets

The datasets from the UNSODA (Unsaturated Soil hydraulic Database, Nemes et al., 2001) were applied to evaluate the model performance. Since the measured SWRC should cover very dry range, a lower boundary of -1.0×10^4 cm were selected for the measured matric potential, resulting in a total of 159 soil samples.

3. Results and Discussions

3.1. Prediction of the hydraulic conductivities with the matching point of K_s

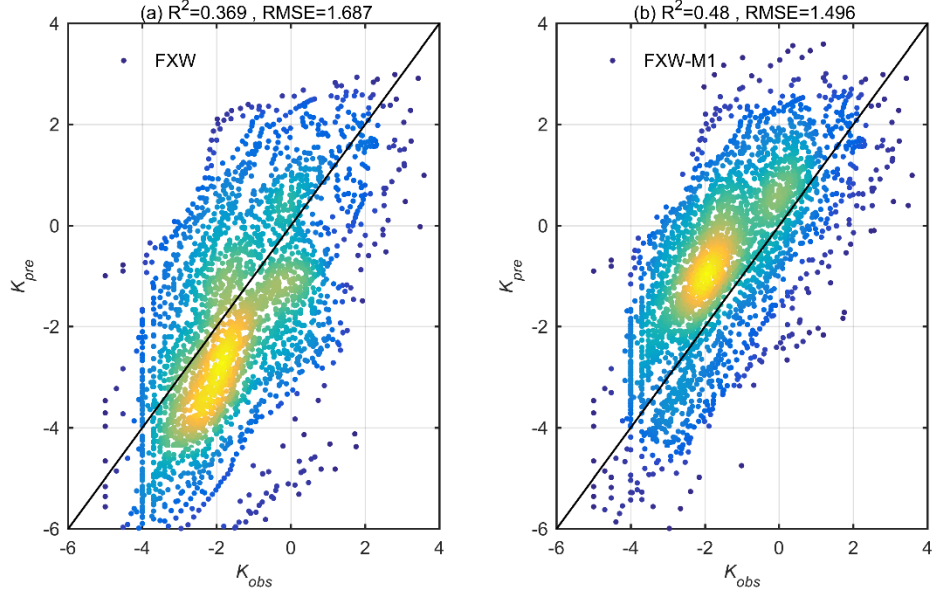


Figure 3. Predicted hydraulic conductivities with the input of K_s . The data density was represented with different color.

Figure 3 presents the predicted hydraulic conductivities with the input of the saturated hydraulic conductivity K_s . Different than in Wang et al. (2018) where a low limit of 1.2 was set for the parameter n , here a value of 1.01 was applied for better describing the SWRC. The original FXW model provided in Wang et al. (2018) performed relatively poor in predicting the HCC (Figure 3 a), with R^2 and $RMSE_{\log_{10}K}$ being 0.37 and 1.69 cm d⁻¹, respectively. It significantly underestimated the conductivity for most datasets. This is different from the findings that found by Schapp and Leij (2000) and Schaap et al. (2001), where applying K_s as the matching point for the VGM model generally led to

overpredicted hydraulic conductivity at most matric potentials. This difference is because nearly half of the evaluated soils here have a small n value close to 1 when fitting SWRC. For this small n , the predictions with the original HCC (equation 1) would drop dramatically just below saturation as shown in Figure 1 (b) and (d), thus underestimated the conductivity.

By introducing a non-zero air-entry value, the modified FXW-M1 model slightly improved the performance in compared with the original FXW model (Figure 3 b). The R^2 increased from 0.37 to 0.48, and the $RMSE_{\log_{10}K}$ reduced from 1.69 to 1.50 cm d⁻¹. Nevertheless, the modified FXW-M1 model with the matching point of K_s still overpredicted the conductivities for most datasets, be in consistent with the findings in Schapp and Leij (2000) and Schaap et al. (2001). This overprediction can be explained as the presence of the macropores near saturation while the matrix flow is controlled by the micropores (Schaap & van Genuchten, 2006).

3.2. Prediction of the hydraulic conductivities with new matching point

The predicted hydraulic conductivities with the new matching point of $K(h_m)$ improved significantly compared to that with the input of K_s . The overall $RMSE_{\log_{10}K}$ and R^2 of the termed FXW-M2 model is 0.84 cm d⁻¹ and 0.74, nearly half and double of the value predicted with the FXW-M1 model, respectively. Figure 4 showed that the predictions were generally close to the observations in the medium range while presented underpredictions in both the wet and dry ends. Further analysis suggested that the underestimation in the wet end happened mainly for the datasets with fitted parameter n value less than 1.1 (Figure 4 b), which was generally for relatively fine-textured soils with wide soil particle size distribution. The inflexion point located approximately at the observed conductivity of 0.1 cm d⁻¹, of which the corresponding matric potential was in the magnitude of tens of centimeters.

Figure 4 shows the predicted hydraulic conductivities with the input of the estimated $K(h_m)$, as well as the fitted water content with equation (2). The fitted water contents were in excellent agreement with observations, the $RMSE$ is 0.014 and the R^2 is 0.99.

Figure 5 shows the predicted conductivities for different soil types. Except for Sand and Sandy loam, almost all soil types exhibited an underprediction in the wet range. The lowest $RMSE_{\log_{10}K}$ of 0.64 cm d⁻¹ was for Silty loam while the worst performance happened for Silty clay, with $RMSE_{\log_{10}K}$ being 1.1 cm d⁻¹ and R^2 being 0.41 (Figure 5 e). For the other soil types, the FXW-M2 model yielded a similar performance.

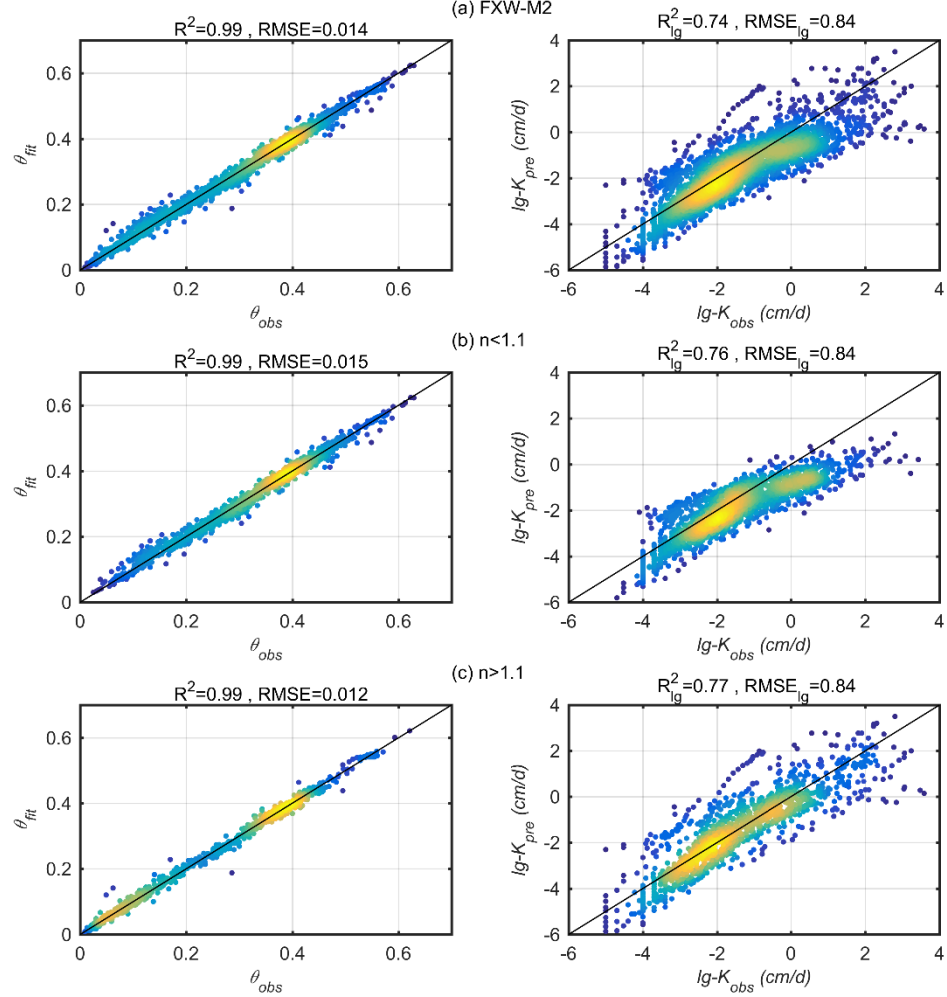


Figure 4. Model performance of the FXW-M2 model. The hydraulic conductivity was predicted totally from the SWRC without the information of K_s .

The noticed underprediction for relatively fine-textured soils could be attributed to the uncertainties in estimating $K(h_m)$. The estimated $K(h_m)$ relies on the accurate estimation of film thickness and the specific surface area. The determination of these two factors, however, could be impacted by many factors, such as the applied value of the Hamaker constant and the ionic concentration (Tokunaga, 2009; 2011). For example, Wang et al. (2017) discussed the impact of different Hamaker constant, which is essentially different for different soil samples (Tuller & Or, 2005; Resurreccion et al., 2011), on specific surface area

and then on the film conductivity estimation. In addition, the possible water retained in very fine pores by the capillarity force may also have a contribution to the conductivity, which, however, was neglected in estimating $K(h_m)$. A higher $K(h_m)$ estimation is expected to improve the predictions of hydraulic conductivities for especially fine-textured soils.

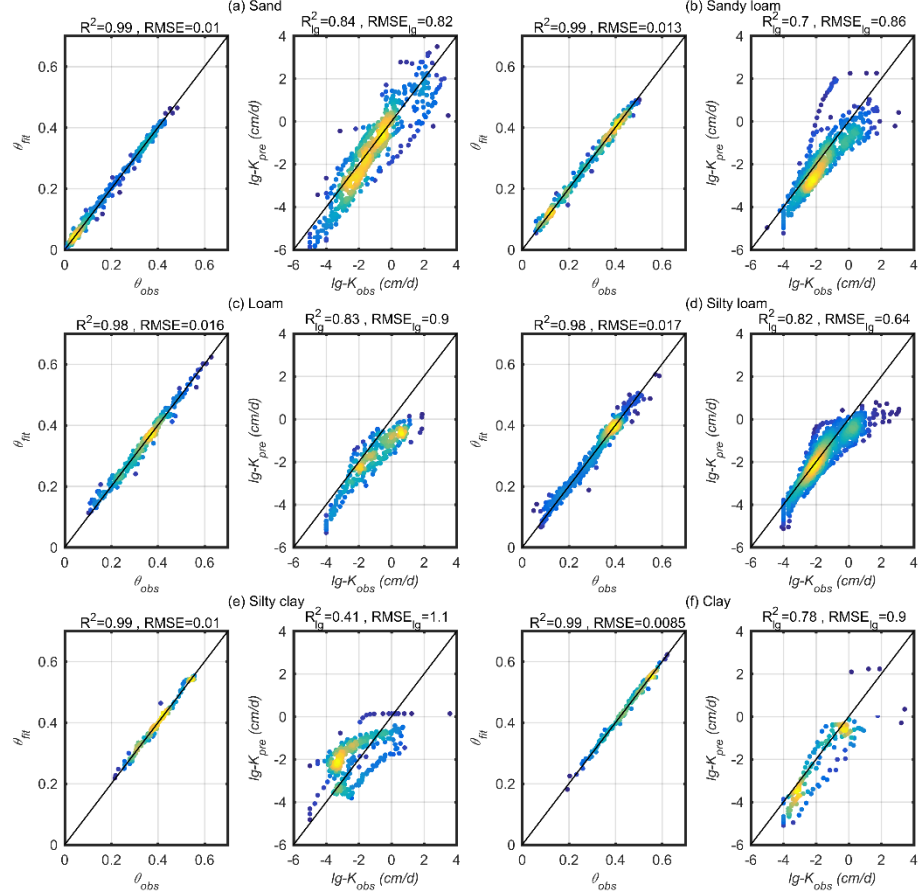


Figure 5. Predicted HCC with FXW-M2 model for different soil types

The sole impact of uncertainty in $K(h_m)$ estimation, however, was not enough to explain the deviation between the predictions and observations. According to equation (14), the hydraulic conductivity is linear with the estimated $K(h_m)$. A higher $K(h_m)$ thus means higher predicted conductivities over the entire matric potential range. Figures 4 and 5, however, indicated that the underprediction only occurred in the wet and dry ends.

Another uncertainty comes from parameter l . Here, a constant value of 3.5 as suggested by Wang et al. (2018) was applied for all soils in predicting the hydraulic conductivities. For different soils, this parameter, however, could have different values. For example, Wang et al. (2018) indicated that a smaller value of 2.8 for l could better describe the conductivities for loam soil.

Overall, the FXW-M2 model performed very well in predicting the HCCs in compared with other models that applied the saturated hydraulic conductivity as matching point. Meanwhile, it required no measured conductivity as matching point and thus was very easy to apply.

To apply this method, the SWRC, however, should cover measurements in very dry range. When there is no direct observation, the water content at h_m can still be predicted from the soil texture information. For example, several empirical relationships had been built between the clay fraction and the SWRC that accounts for the dry range (e.g., Resurreccion et al., 2011; Schneider & Goss, 2012; Arthur et al., 2013).

3.3. Optimized parameters $b(h_m)$ and l

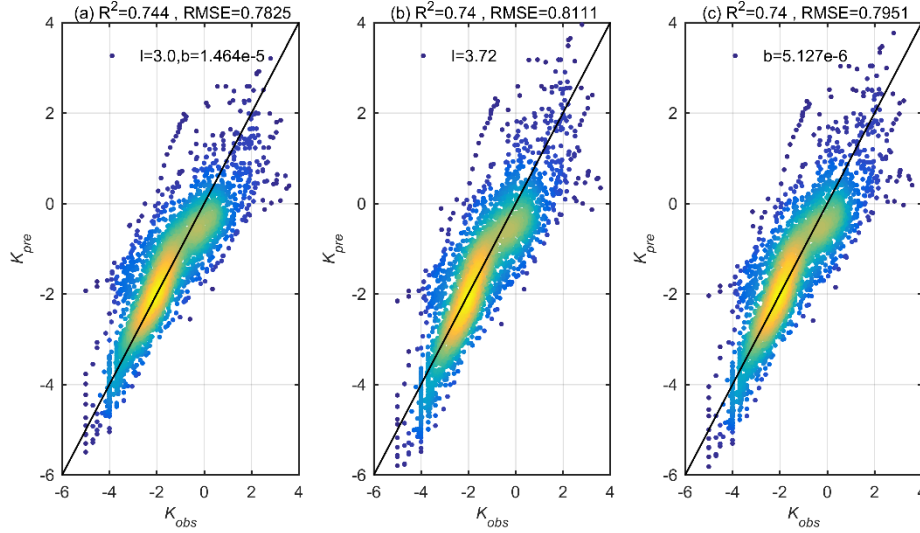


Figure 6. The predicted conductivities with optimized l and $b(h_m)$. (a) means both two parameters were optimized while (b) and (c) represents the results with solely optimized l and $b(h_m)$, respectively.

Figure 6 (a) showed the predicted conductivities with optimized l and $b(h_m)$. Testing with 159 soil samples yielded the optimized value was 3.0 for parameter l and $1.464 \times 10^{-5} \text{ cm d}^{-1}$ for $b(h_m)$, respectively. The optimized $b(h_m)$ was about 5 times of the theoretical value estimated in section 2.2. This may indicate that the method presented in section 2.2 underestimated the $K(h_m)$ for especially fine-textured soils. Interestingly, the optimized l value is the same as the one

suggested by Rudiyanto et al. (2020). With the optimized parameters l and $b(h_m)$, the FXW-M2 model improved the predictions in both the wet and dry end, with $RMSE_{\log_{10}K}$ reducing from 0.84 to 0.78 cm d⁻¹. Also shown in Figure 6 (b) and (c) were the results with solely optimized l and $b(h_m)$, respectively. The results indicated that the predicted conductivities were mainly impacted by the parameter of $b(h_m)$.

4. Concluding Remarks

In this study, we developed a modified form of the HCC model that provided by Wang et al. (2018) to overcome the abrupt drop of hydraulic conductivity near saturation for small n values. This is achieved by introducing a non-zero air-entry value following Vogel et al. (2000) and Ippisch et al. (2006). Compared to the original FXW model, the modified model, termed as FXW-M1 model, improved the prediction of conductivities with the input of saturated conductivity.

By applying an estimated conductivity at dry range as matching point, we further modified the FXW-M1 model to eliminate the parameter of the saturated hydraulic conductivity. The resulting FXW-M2 model can predict the HCC totally from SWRC, requiring no additional information. The new model significantly improved the predictions of hydraulic conductivity, with the root mean value about a half of that with the input of saturated hydraulic conductivity. Therefore, it provided an easy and accurate way for predicting the hydraulic conductivity information, which would facilitate the water and solute transport simulation in land surface modelling.

Acknowledgments

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